

* * * * * Welcome to STN International * * * * *

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 and searchable
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
 CA/CAPLUS
NEWS 5 FEB 05 German (DE) application and patent publication number format
 changes
NEWS 6 MAR 03 MEDLINE and LMEADLINE reloaded
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 8 MAR 03 FRANCEPAT now available on STN
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
NEWS 10 MAR 29 WPIFV now available on STN
NEWS 11 MAR 29 No connect hour charges in WPIFV until May 1, 2004
NEWS 12 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

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STRUCTURE FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6

DICTIONARY FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

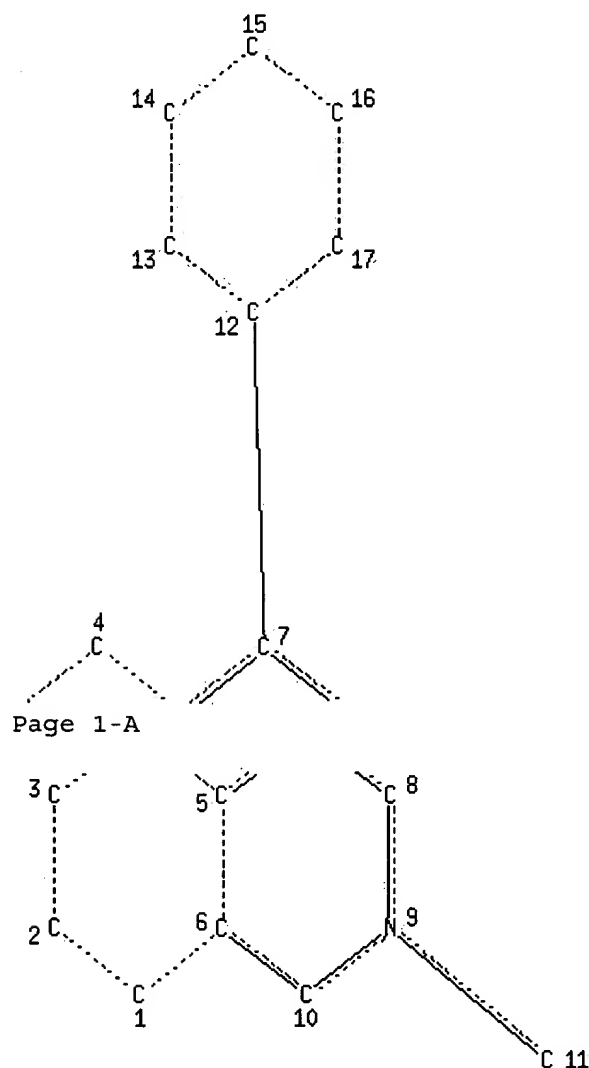
=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Page 1-A

Page 2-A

NODE ATTRIBUTES:

NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5

NSPEC IS R AT 6
 NSPEC IS R AT 7
 NSPEC IS R AT 8
 NSPEC IS R AT 9
 NSPEC IS R AT 10
 NSPEC IS RC AT 11
 NSPEC IS R AT 12
 NSPEC IS R AT 13
 NSPEC IS R AT 14
 NSPEC IS R AT 15
 NSPEC IS R AT 16
 NSPEC IS R AT 17
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 11
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 12
 NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 20:07:30 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 3117 TO ITERATE

32.1% PROCESSED 1000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

34 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 58992 TO 65688
 PROJECTED ANSWERS: 1502 TO 2736

L2 34 SEA SSS SAM L1

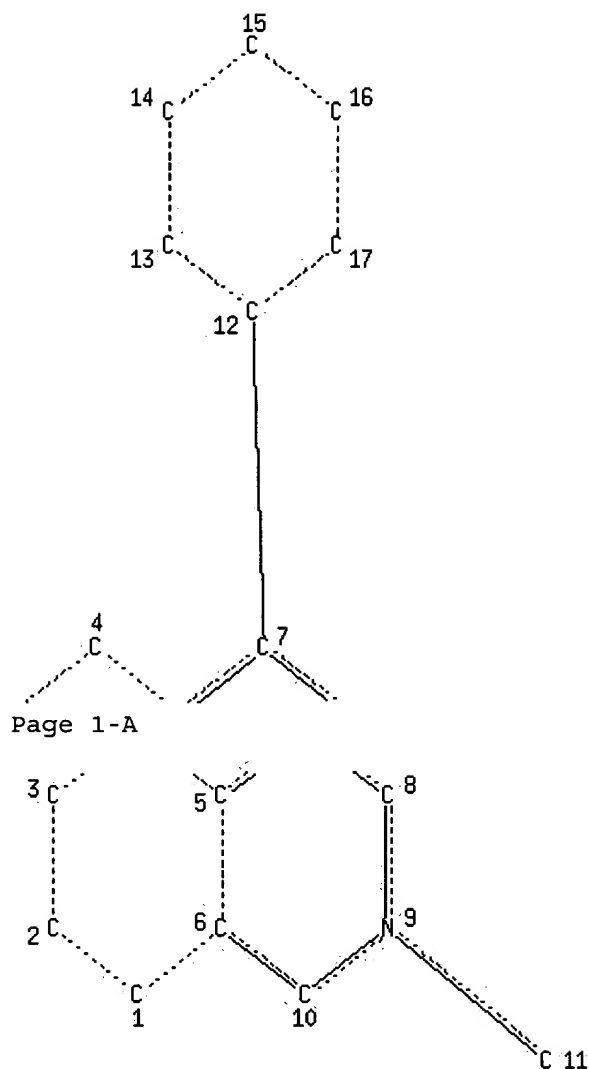
=>

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



Page 2-A

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS RC	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS R	AT	17

DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 11
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

=> s 13

SAMPLE SEARCH INITIATED 20:08:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3117 TO ITERATE

32.1% PROCESSED 1000 ITERATIONS 30 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58992 TO 65688
PROJECTED ANSWERS: 1290 TO 2450

L4 30 SEA SSS SAM L3

=> s 13 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:08:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62007 TO ITERATE

100.0% PROCESSED 62007 ITERATIONS 1786 ANSWERS
SEARCH TIME: 00.00.01

L5 1786 SEA SSS FUL L3

=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

L1 STRUCTURE UPLOADED
L2 34 S L1
L3 STRUCTURE UPLOADED
L4 30 S L3
L5 1786 S L3 FULL

=> s 12 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:08:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62007 TO ITERATE

100.0% PROCESSED 62007 ITERATIONS 2027 ANSWERS
SEARCH TIME: 00.00.01

L6 2027 SEA SSS FUL L1

=> s 16 not 15

L7 241 L6 NOT L5

=>

L8 STRUCTURE UPLOADED

=> l8

L8 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

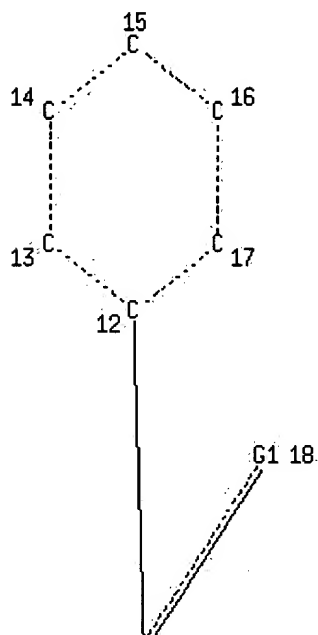
=> d l8

L8 HAS NO ANSWERS

L8 STR

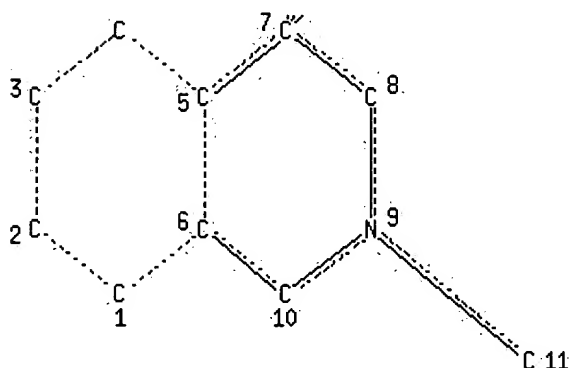
H 19 0 20 S 21 X 22

Page 1-A



4

Page 1-B



Page 2-B

VAR G1=19/20/21/22

NODE ATTRIBUTES:

NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10

```

NSPEC  IS RC      AT  11
NSPEC  IS R       AT  12
NSPEC  IS R       AT  13
NSPEC  IS R       AT  14
NSPEC  IS R       AT  15
NSPEC  IS R       AT  16
NSPEC  IS R       AT  17
NSPEC  IS C       AT  18
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  11 19 20 21 22
DEFAULT ECLEVEL IS LIMITED

```

GRAPH ATTRIBUTES:

```

RSPEC  12
NUMBER OF NODES IS  22

```

STEREO ATTRIBUTES: NONE

=> s l8

```

SAMPLE SEARCH INITIATED 20:10:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3117 TO ITERATE

```

```

32.1% PROCESSED      1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

```

33 ANSWERS

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:    58992 TO    65688
PROJECTED ANSWERS:       1449 TO    2665

```

L9 33 SEA SSS SAM L8

=> s l8 full

```

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:10:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62007 TO ITERATE

```

```

100.0% PROCESSED      62007 ITERATIONS
SEARCH TIME: 00.00.01

```

1889 ANSWERS

L10 1889 SEA SSS FUL L8

=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

```

L1          STRUCTURE UPLOADED
L2          34 S L1
L3          STRUCTURE UPLOADED
L4          30 S L3
L5          1786 S L3 FULL
L6          2027 S L2 FULL
L7          241 S L6 NOT L5
L8          STRUCTURE UPLOADED
L9          33 S L8
L10         1889 S L8 FULL

```

=> s l10 not l5
 L11 211 L10 NOT L5

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	468.36	468.57

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004
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FILE COVERS 1907 - 14 Apr 2004 VOL 140 ISS 16
 FILE LAST UPDATED: 13 Apr 2004 (20040413/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11
 L12 24 L11

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	470.93

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004
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STRUCTURE FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6
 DICTIONARY FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer

to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

```
L1          STRUCTURE UPLOADED
L2          34 S L1
L3          STRUCTURE UPLOADED
L4          30 S L3
L5          1786 S L3 FULL
L6          2027 S L2 FULL
L7          241 S L6 NOT L5
L8          STRUCTURE UPLOADED
L9          33 S L8
L10         1889 S L8 FULL
L11         211 S L10 NOT L5
```

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004

```
L12         24 S L11
```

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 20:11:40 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 62007 TO ITERATE

```
100.0% PROCESSED    62007 ITERATIONS                1786 ANSWERS
SEARCH TIME: 00.00.01
```

```
L13         1786 SEA SSS FUL L3
```

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	626.35

FILE 'HCAPLUS' ENTERED AT 20:11:45 ON 14 APR 2004

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FILE COVERS 1907 - 14 Apr 2004 VOL 140 ISS 16
 FILE LAST UPDATED: 13 Apr 2004 (20040413/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

```
L1          STRUCTURE UPLOADED
L2          34 S L1
L3          STRUCTURE UPLOADED
L4          30 S L3
L5          1786 S L3 FULL
L6          2027 S L2 FULL
L7          241 S L6 NOT L5
L8          STRUCTURE UPLOADED
L9          33 S L8
L10         1889 S L8 FULL
L11         211 S L10 NOT L5
```

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004

```
L12         24 S L11
```

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004

```
L13         1786 S L4 FULL
```

FILE 'HCAPLUS' ENTERED AT 20:11:45 ON 14 APR 2004

=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

```
L1          STRUCTURE UPLOADED
L2          34 S L1
L3          STRUCTURE UPLOADED
L4          30 S L3
L5          1786 S L3 FULL
L6          2027 S L2 FULL
L7          241 S L6 NOT L5
L8          STRUCTURE UPLOADED
L9          33 S L8
L10         1889 S L8 FULL
L11         211 S L10 NOT L5
```

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004

```
L12         24 S L11
```

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004

```
L13         1786 S L4 FULL
```

FILE 'HCAPLUS' ENTERED AT 20:11:45 ON 14 APR 2004

=> s l12 and beck, j?/au

```
1487 BECK, J?/AU
```

```
L14         1 L12 AND BECK, J?/AU
```

=> d l14, ibib abs fhitrstr, 1

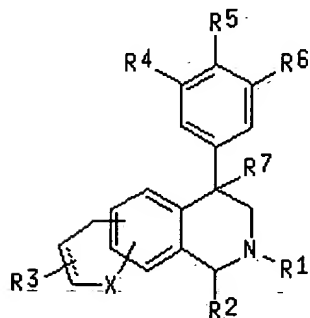
L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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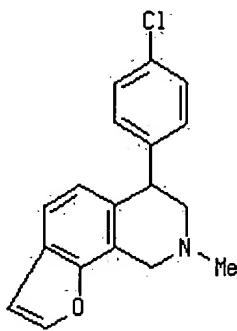
ACCESSION NUMBER: 2002:51467 HCAPLUS
DOCUMENT NUMBER: 136:118393
TITLE: Preparation and use of furan-fused-4-phenyl substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD)
INVENTOR(S): Beck, James P.; Pechulis, Anthony D.; Harms, Arthur E.
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004455	A2	20020117	WO 2001-US21818	20010711
WO 2002004455	A3	20020620		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002091134	A1	20020711	US 2001-902845	20010711
EP 1299393	A2	20030409	EP 2001-952616	20010711
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001012350	A	20030624	BR 2001-12350	20010711
JP 2004502774	T2	20040129	JP 2002-509320	20010711
PRIORITY APPLN. INFO.:				
			US 2000-217412P	P 20000711
			WO 2001-US21818	W 20010711

OTHER SOURCE(S): MARPAT 136:118393
GI



I



II

AB Title compds. I [R1 = alk(en/yn)yl, cycloalkyl, 5-cycloalkylalkyl and benzyl, each of which is optionally substituted with 1 to 3 substituents; R2 = H, alk(en/yn)yl, cycloalkyl, cycloalkylalkyl and haloalkyl; R3 = H, halo, alkyl, haloalkyl and cycloalkyl, wherein alkyl, haloalkyl and

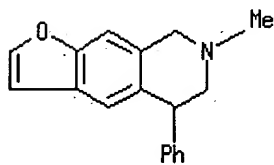
cycloalkyl are optionally substituted with 1 to 3 substituents selected from alkoxy and amino; R4-6 = H, halo, alkoxy, NO₂, amino, amido, ureido, S(O)_n, CN, acyl, carboxy, carboxamide, alk(en/yn)yl, cycloalkyl and cycloalkylalkyl; alternatively R5-6 = O-alkyl-O; R7 = H, halo and alkoxy; X = O, NH (and substituted derivs.) and S; n = 0 - 2] with some provisos, were prepd. E.g., 7-formylbenzofuran was converted to the corresponding methylamino-Me deriv. (MeOH, MeNH₂, NaBH₄), alkylated with p-chlorophenacyl bromide (CH₂Cl₂, Et₃N) and reduced to the amino alc. (CH₂Cl₂, NaBH₄, 5 h, 0° → room temp.). This intermediate was treated dropwise with MsOH (CH₂Cl₂, 0°C → reflux, overnight) to give II as a yellow oil (18% overall yield). Over 150 synthetic examples were provided. Compds. I are selective neurotransmitter receptor binding ligands (no data). I are useful in the treatment of attention-deficit hyperactivity disorder.

IT 389845-75-4P

RL: BYP (Byproduct); PREP (Preparation)
(byproduct; prepn. and use of furan-fused-4-Ph substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD))

RN 389845-75-4 HCAPLUS

CN Furo[3,2-g]isoquinoline, 5,6,7,8-tetrahydro-7-methyl-5-phenyl- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

L1 STRUCTURE UPLOADED
L2 34 S L1
L3 STRUCTURE UPLOADED
L4 30 S L3
L5 1786 S L3 FULL
L6 2027 S L2 FULL
L7 241 S L6 NOT L5
L8 STRUCTURE UPLOADED
L9 33 S L8
L10 1889 S L8 FULL
L11 211 S L10 NOT L5

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004

L12 24 S L11

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004

L13 1786 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 20:11:45 ON 14 APR 2004

L14 1 S L12 AND BECK, J?/AU

=> s l12 not l14

L15 23 L12 NOT L14

```
=> s l15 and pechulis, a?/au
      8 PECHULIS, A?/AU
L16      0 L15 AND PECHULIS, A?/AU
```

```
=> s l15 and harms, a?/au
      225 HARMS, A?/AU
L17      0 L15 AND HARMS, A?/AU
```

```
=> file caold
COST IN U.S. DOLLARS                SINCE FILE      TOTAL
                                     ENTRY      SESSION
FULL ESTIMATED COST                9.48      635.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                             ENTRY      SESSION
CA SUBSCRIBER PRICE                -0.69      -0.69
```

FILE 'CAOLD' ENTERED AT 20:12:41 ON 14 APR 2004
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

```
=> d his
```

(FILE 'HOME' ENTERED AT 20:06:03 ON 14 APR 2004)

FILE 'REGISTRY' ENTERED AT 20:06:13 ON 14 APR 2004

```
L1      STRUCTURE UPLOADED
L2      34 S L1
L3      STRUCTURE UPLOADED
L4      30 S L3
L5      1786 S L3 FULL
L6      2027 S L2 FULL
L7      241 S L6 NOT L5
L8      STRUCTURE UPLOADED
L9      33 S L8
L10     1889 S L8 FULL
L11     211 S L10 NOT L5
```

FILE 'HCAPLUS' ENTERED AT 20:11:06 ON 14 APR 2004

```
L12      24 S L11
```

FILE 'REGISTRY' ENTERED AT 20:11:32 ON 14 APR 2004

```
L13      1786 S L4 FULL
```

FILE 'HCAPLUS' ENTERED AT 20:11:45 ON 14 APR 2004

L14 1 S L12 AND BECK, J?/AU
 L15 23 S L12 NOT L14
 L16 0 S L15 AND PECHULIS, A?/AU
 L17 0 S L15 AND HARMS, A?/AU

FILE 'CAOLD' ENTERED AT 20:12:41 ON 14 APR 2004

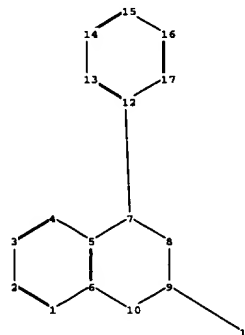
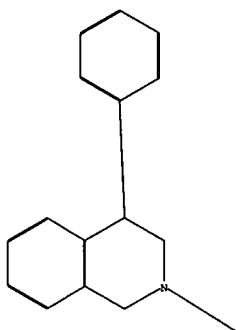
=> s l11

L18 0 L11

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	636.25
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.69

STN INTERNATIONAL LOGOFF AT 20:13:22 ON 14 APR 2004



ring nodes :

1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17

ring/chain nodes :

11

chain bonds :

7-12 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

5-7 6-10 7-8 8-9 9-10 9-11

exact bonds :

7-12

normalized bonds :

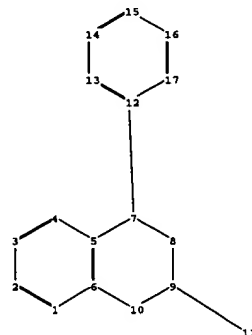
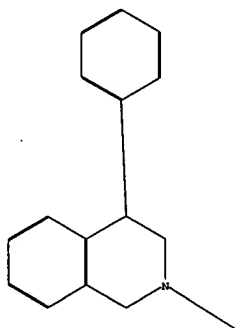
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 12 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom



ring nodes :

1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17

ring/chain nodes :

11

chain bonds :

7-12 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

5-7 6-10 7-8 8-9 9-10 9-11

exact bonds :

7-12

normalized bonds :

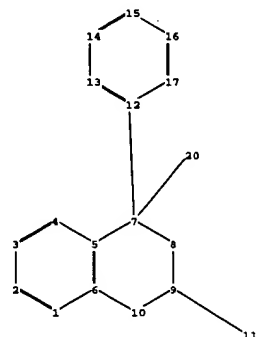
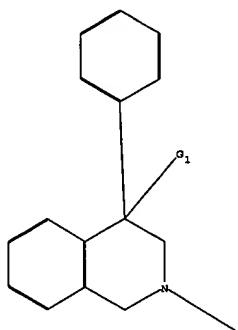
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 1 : 12 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom



chain nodes :

20

ring nodes :

1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17

ring/chain nodes :

11

chain bonds :

7-12 7-20 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

5-7 6-10 7-8 7-20 8-9 9-10 9-11

exact bonds :

7-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 12 :

G1:H,O,S,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 20:CLASS